Fully Quantum Calculation of Dielectric Virial Coefficients for Molecular Gases

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We present our recent results on the *ab-initio* calculation of dielectric virial coefficients of molecular systems; building on our previous results for noble gases, we developed a systematic path-integral approach that can in principle be applied to coefficients of any order.

This approach is validated by computing the contributions to the first virial coefficient of water vapor due to the electronic polarizability and the dipole-moment surface. The latter contribution can also be computed from spectroscopic information available from the HITRAN2020 database, and we find a very good agreement. Our approach points out limitations of the current polarizability and dipole-moment surface for water, in particular the lack of a well-defined uncertainty estimation.

In the case of higher-order dielectric virial coefficients, our approach suffers from the current shortage of well-defined ab-initio polarizability and dipole-moment surfaces. Nevertheless, we present results on the second dielectric virial coefficient based on physically motivated approximations.